

Application No.: 09/915,515

Docket No.: 21663-00193-US

AMENDMENTS TO THE CLAIMS

1. (Previously presented) A method for identifying a potential inhibitor for a paramyxovirus Hemagglutinin-neuraminidase, comprising:
 - a. applying a three-dimensional structure of the paramyxovirus Hemagglutinin-neuraminidase as defined by the structure coordinates comprising the amino acid residues 174, 175, 190, 192, 199, 234, 236, 237, 254, 256, 258, 262, 299, 302, 317, 363, 364, 369, 401, 416, 466, 498, and 526 according to SEQ ID NO: 1 to design or select the potential inhibitor;
 - b. obtaining the potential inhibitor; and
 - c. associating the potential inhibitor with the enzyme in the presence of a substrate to determine the ability of the potential inhibitor to inhibit the enzyme.
2. (Original) The method according to claim 1, wherein the potential inhibitor is designed de novo.
3. (Original) The method according to claim 1, wherein the potential inhibitor is designed from a known inhibitor.
4. (Previously presented) The method according to claim 1, wherein applying the three-dimensional structure to design or select the compound comprises
 - a. identifying chemical entities or fragments capable of associating with the enzyme; and
 - b. assembling the identified chemical entities or fragments into a single molecule to provide the structure of the potential inhibitor.
5. (Original) The method of according to claim 4, wherein the potential inhibitor is designed de novo.
6. (Original) The method according to claim 4, wherein the potential inhibitor is designed from a known inhibitor.

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7. (Withdrawn) A complex of a paramyxovirus Hemagglutinin-neuraminidase and a substrate or inhibitor molecule.

8. (Withdrawn) The complex of claim 7 being obtained by diffusion or co-crystallization.

9. (Previously presented) The method according to claim 1 wherein the potential inhibitor is a competitive, noncompetitive, or uncompetitive inhibitor of a paramyxovirus Hemagglutinin neuraminidase.

10. (Previously presented) The method according to claim 1 wherein the potential inhibitor is designed to form salt links with Arg416 and Arg498 of a paramyxovirus Hemagglutinin neuraminidase.

11. (Withdrawn) The method according to claim 1 wherein the potential inhibitor is designed to form hydrogen bonds or salt links with Glu258 of a paramyxovirus Hemagglutinin neuraminidase.

12. (Currently amended) The method according to claim 1 wherein the potential inhibitor is designed to form hydrogen bonds or salt links with Lys 236 499 of a paramyxovirus Hemagglutinin neuraminidase.

13. (Canceled)

14. (Previously presented) The method of claim 1 wherein the paramyxovirus hemagglutinin-neuraminidase is Newcastle Disease Virus Hemagglutinin neuraminidase.

15. (Withdrawn) A machine readable data storage medium comprising a data storage material encoded with machine-readable data which comprises the structure coordinates

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comprising the amino acid residues 174, 175, 190, 192, 199, 234, 236, 237, 254, 256, 258, 262, 299, 302, 317, 363, 364, 369, 401, 416, 466, 498 and 526 according to SEQ ID NO:1.

16. (Withdrawn) The machine-readable data storage medium of claim 15 wherein the machine-readable data comprises the three-dimensional structure of paramyxovirus Hemagglutinin-neuraminidase.

17. (Withdrawn) The machine-readable data storage medium of claim 16 wherein the paramyxovirus Hemagglutinin-neuraminidase is Newcastle Disease Virus Hemagglutinin-Neuraminidase.

18. (Withdrawn) A computer for producing a three-dimensional representation of:

- a. a molecule or molecular complex, wherein said molecules or molecular complex comprises a binding pocket defined by structure coordinates comprising the amino acid residues 174, 175, 190, 192, 199, 234, 236, 237, 254, 256, 258, 262, 299, 302, 317, 363, 364, 369, 401, 416, 466, 498 and 526 according to SEQ ID NO:1; wherein the computer comprises:
 - (i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, comprising the structure coordinates comprising the amino acid residues 174, 175, 190, 192, 199, 234, 236, 237, 254, 256, 258, 262, 299, 302, 317, 363, 364, 369, 401, 416, 466, 498 and 526 according to SEQ ID NO:1;
 - (ii) a working memory for storing instructions for processing the machine-readable data;
 - (iii) a central-processing unit coupled to the working memory and to the machine-readable data storage medium for processing the machine readable data into the three-dimensional representation; and
 - (iv) a display coupled to the central-processing unit for displaying the three-dimensional representation.

19. (Withdrawn) The computer of claim 18 wherein the computer produces a three-dimensional representation of a paramyxovirus Hemagglutinin-neuraminidase; and

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wherein the machine-readable data comprises the structure coordinates of paramyxovirus Hemagglutinin-neuraminidase.

20. (Withdrawn) The computer of claim 18 wherein the computer produces a three-dimensional representation of Newcastle Disease Virus Hemagglutinin Neuraminidase and wherein the machine readable data comprises the structure coordinate of Newcastle Disease Virus Hemagglutinin Neuraminidase.

21. (Original) The method of claim 1 which comprises:
employing computational means to perform a fitting operation between the potential inhibitor and the structure coordinates of the three-dimensional structure; and
analyzing the results of the fitting operation to quantify the association between the potential inhibitor and the structure coordinates.